

FIG. 1

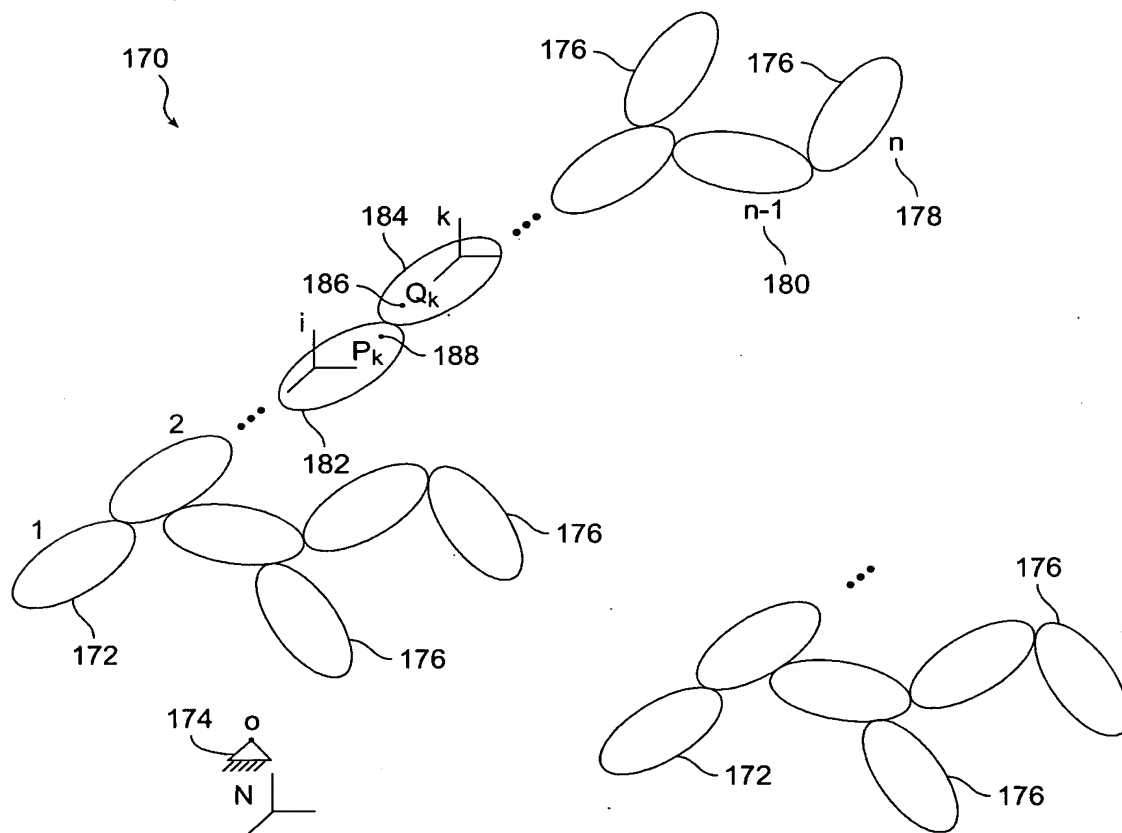


FIG. 2

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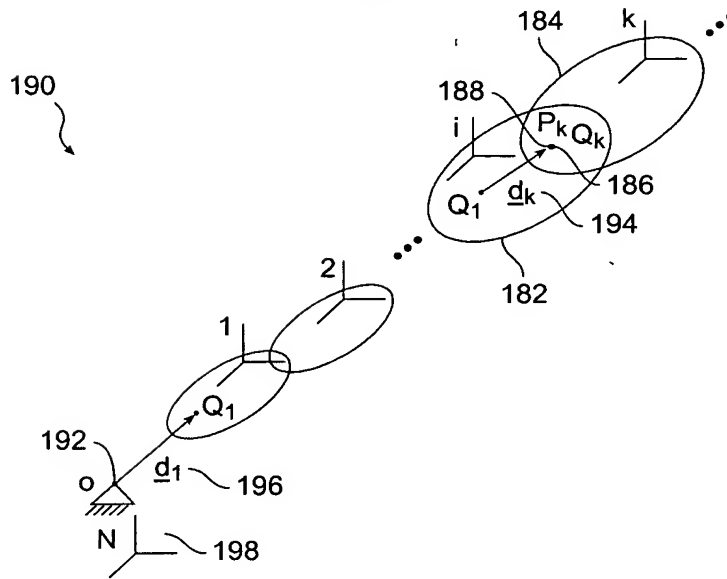


FIG. 3

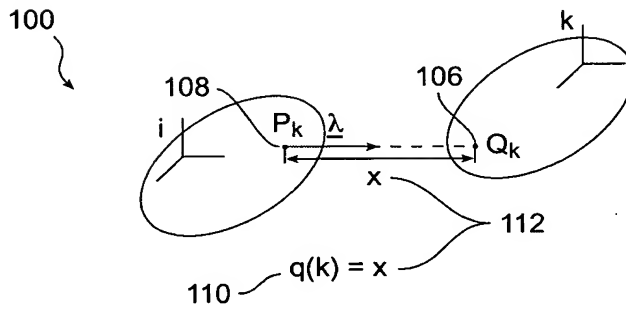


FIG. 4A

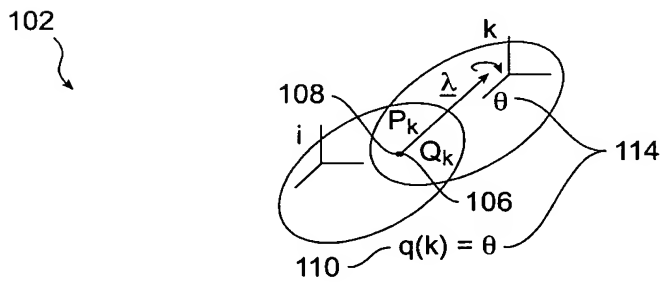


FIG. 4B

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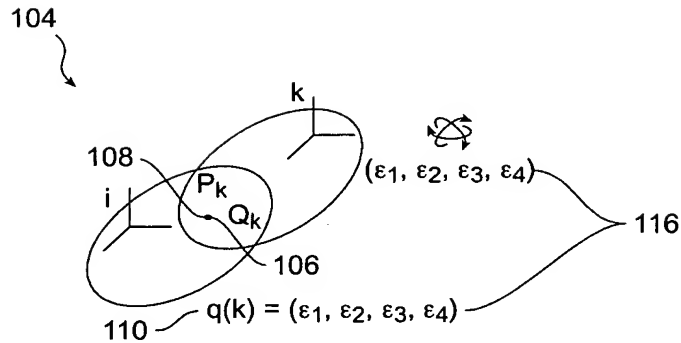


FIG. 4C

RESIDUAL FORM METHOD TO COMPUTE ρ_q AND ρ_u	DIRECT FORM METHOD TO COMPUTE \dot{q} AND \dot{u}
<ol style="list-style-type: none"> 1. COMPUTE THE FIRST KINEMATICS CALC. AND THE FIRST KINEMATIC RESIDUAL $\rho_q(k)$ 2. GENERATE $\hat{T}(k)$, THE SPACIAL LOAD BALANCE FOR EACH BODY 3. COMPUTE DYNAMIC RESIDUAL $\rho_u(k)$ 	<ol style="list-style-type: none"> 1. COMPUTE \dot{q} USING JOINT SPECIFIC ROUTINES 2. PERFORM FIRST KINEMATICS CALC. WITH $\dot{u} = 0$ 3. GENERATE RESIDUALS ρ_u AND NEGATE $\rho_u = -\rho_u$ 4. PERFORM SECOND KINEMATICS CALC. 5. COMPUTE \dot{u} USING FORWARD DYNAMICS

COMPARISON OF METHODS

FIG. 5



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MOLECULE	NO. RESIDUES IN POLYPEPTIDE	NO. ATOMS	DIRECT FORM APPROXIMATE OPERATION COUNT	RESIDUAL FORM APPROXIMATE OPERATION COUNT	FACTOR OF SPEED UP
ALANINE DIPEPTIDE	2	23	4,991	683	7.31
20-MER POLYALANINE	20	257	42,340	5,894	7.24
100-MER POLYALANINE	100	1297	207,018	28,973	7.15

COMPUTATION COMPARISON

FIG. 6